Accurate Thermophysical Characterization of Aqueous Systems with the Soft-SAFT Equation of State

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Water is probably the most fundamental building block of life on Earth. However, the apparently simple structure of this compound exhibits highly complex and non-ideal behaviour both as a pure fluid and in mixtures. The main reason for this complexity is the associating nature of this compound – the anisotropic hydrogen bonding observed in H_2O exerts an important influence on its thermophysical properties and phase behaviour. Hence, the description of the thermophysical properties of aqueous mixtures is an important challenge for any equation of state. Considering that aqueous mixtures are found in almost all industrial processes, reliable tools capable of providing an accurate description of the thermophysical properties are in high demand. In this contribution, we present new models developed using the soft-SAFT EoS to describe the thermophysical properties of a number of aqueous systems of industrial interest, with particular emphasis on water + CO_2, water + 1-alkanols and water + ionic liquids. The vapour-liquid and liquid-liquid equilibria of these systems are described in a wide range of temperatures and pressures in good agreement with the experimental data. The calculation of the interfacial tension of some of these mixtures is also included by coupling a Density Gradient Approach into soft-SAFT. In a similar manner, the viscosity of these mixtures is also calculated using the Free-Volume-Theory (FVT). This study is finally completed by the calculation of some derivative properties and excess properties of interest.

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